

THE CRYSTAL AND MOLECULAR STRUCTURE OF *L*-ORNITHINE-HYDROCHLORIDE

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CALCUTTA-9.

(Received August 10, 1967)

Ornithine—a lower homologue of lysine—plays an important role in the formation of urea in the body. This communication deals with the crystal structure of a derivative of ornithine, $C_5H_{12}N_2O_2 \cdot HCl$ (Saha *et al.*, 1966). A preliminary report on this structure was presented at the symposium of the Indian Biophysical Society in April, 1967.

Ornithine hydrochloride crystallises in the monoclinic system with cell dimensions; $a = 4.99 \text{ \AA}$; $b = 8.00 \text{ \AA}$; $c = 10.00 \text{ \AA}$; $\beta = 97.0^\circ$, and space group $P2_1$. The measured density (1.420 g.cm^{-3}) corresponds to two molecules per unit cell, the calculated density being 1.416 g.cm^{-3} .

Three-dimensional intensity data collected about a and b axes by multiple film equi-inclination Weissenberg technique using CuK_α radiation were corrected for spot-size, Lorentz and polarisation factors. The relative intensity values thus obtained for different layers were brought to the same scale by using cross layer correlation method. The positions of two heavy atoms (chlorine) in the unit cell were determined from two Patterson projections, viz. (010) and (100), and a Harker section at $v = \frac{1}{2}$. The structure was solved by (a) a Buerger's minimum function derived from Cl-Cl vector in the three-dimensional Patterson map and (b) a three-dimensional Fourier synthesis based on phase angles of chlorine atoms; both calculated on IBM 1620 computer. Refinement of atomic parameters was made (five cycles) by the method of least squares using isotropic temperature factors and unit weighting factor. The final R value (including unobserved reflections) is 0.098.

The interatomic bond lengths and angles (Table II and Fig. 1) compare well with those of lysine hydrochloride (Wright *et al.*, 1962) and other amino acids (Hahn, 1957). The near equality of the two C—O bond distances (the difference being 0.012 \AA from their average value 1.254 \AA) indicates that the molecule is a zwitterion, both amino and terminal nitrogen atoms accepting a proton each. The average value of the (1.530 \AA) four C—C bond distances, though slightly higher than that of lysine hydrochloride (1.524), agrees well with the ($1.533 \pm 0.003 \text{ \AA}$) found by Bartell (1959) for medium length aliphatic carbon chains. The two

C—N+H₃ bond lengths are almost equal and their average (1.490 Å) compares well with that of lysine hydrochloride (1.482 ± 0.004 Å). Though the average value

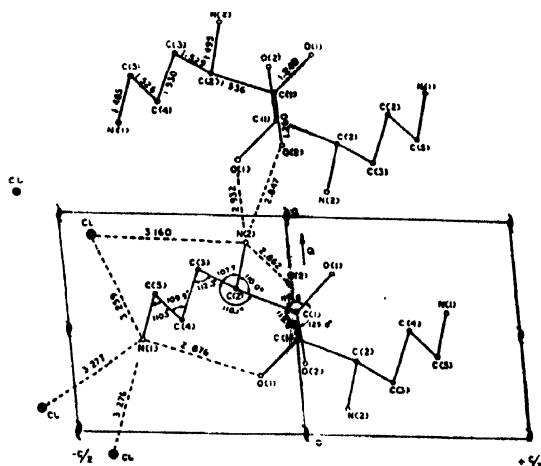


Fig. 1. The structure of L-ornithine hydrochloride viewed down the *b*-axis.

(110.7°) of three C—C—C angles in this molecule is not far from tetrahedral angle, a widening of the C(2)—C(3)—C(4) angle (112.3°) was found.

The molecules are held together by a system of hydrogen bonds. Each molecule has six hydrogen atoms available for hydrogen bond formation. Fig. 1, shows that both amino and terminal nitrogen atoms have four close neighbours each at hydrogen bond forming distances. All the C—NH...X bond angle (Table III) except C(2)—N(2)H...O_V(1) = 166.4° and C(5)—N(1)H...Cl_{IV} = 173.5° satisfy the expected tetrahedral configuration, which indicates that these two sites are not favourable for hydrogen bond formation. The detailed paper on this structure will be published shortly.

TABLE I

Final atomic co-ordinates and temperature factors

Atom	X	Y	Z	B
Cl	0.09701	0.25000	0.41901	2.828
N(1)	0.42113	0.00143	0.64392	2.674
C(5)	0.63620	0.12784	0.67799	2.690
C(4)	0.52069	0.28208	0.74060	2.876
C(3)	0.75135	0.40285	0.78644	2.408
C(2)	0.65798	0.55106	0.86550	2.148
N(2)	0.88871	0.67100	0.88970	2.251
C(1)	0.57395	0.49112	0.00044	2.353
O(1)	0.75608	0.46503	0.09457	3.076
O(2)	0.32598	0.46701	0.00274	2.843

TABLE II
Intramolecular interatomic bond distances and angles

Bond distances		Bond angles	
N(1)—C(5)	1.485 Å	N(1)—C(5)—C(4)	110.3°
C(5)—C(4)	1.526 Å	C(5)—C(4)—C(3)	109.9°
C(4)—C(3)	1.530 Å	C(4)—C(3)—C(2)	112.3°
C(3)—C(2)	1.529 Å	C(3)—C(2)—C(1)	110.1°
C(2)—C(1)	1.536 Å	C(3)—C(2)—N(2)	107.7°
C(3)—N(2)	1.495 Å	N(2)—C(2)—C(1)	110.0°
C(1)—O(1)	1.248 Å	C(2)—C(1)—O(1)	117.8°
C(1)—O(2)	1.260 Å	C(2)—C(1)—O(2)	115.9°
		O(1)—C(1)—O(2)	125.8°

TABLE III
Intermolecular bond distances and angles

Bond distances		Bond angles	
N(1)—H...Cl _I	3.277 Å	C(5)—N(1)...Cl _I	91.5°
N(1)—H...Cl _{II}	3.259 Å	C(5)—N(1)...Cl _{II}	86.2°
N(1)—H...O _{II} (1)	2.876 Å	C(5)—N(1)...O _{II} (1)	98.9°
N(2)—H...Cl _V	3.160 Å	C(2)—N(2)...Cl _V	94.5°
N(2)—H...O _V (2)	2.862 Å	C(2)—N(2)...O _V (2)	106.0°
N(2)—H...O _{III} (2)	2.847 Å	C(2)—N(2)...O _{III} (2)	103.5°
N(1)...Cl _{VI}	3.276 Å	C(5)—N(1)...Cl _{VI} (9)	173.5°
N(2)...O _{VI} (1)	2.932 Å	C(2)—N(2)...O _{VI} (1)	166.4°

The subscripts refer to the co-ordinates of atoms in molecules I to VI. I : X, Y, Z; II : —X, Y— $\frac{1}{2}$, —Z; III : —X+1, Y— $\frac{1}{2}$, —Z; IV : —X—1, Y— $\frac{1}{2}$, —Z; V : —X, Y+ $\frac{1}{2}$, —Z; VI : —X+1, Y+ $\frac{1}{2}$, —Z.

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